

Problem 4 (6 Points)

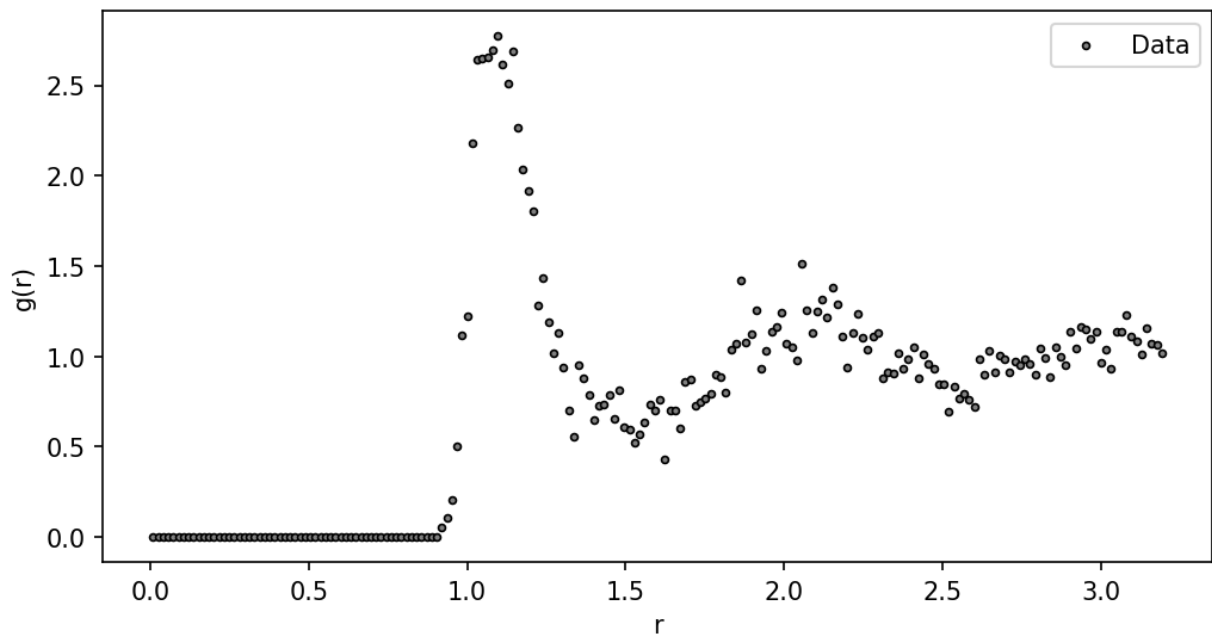
256 particles of liquid argon are simulated at 100K. A radial distribution function $g(r)$ describes the density of particles a distance of r from each particle in the system. When an $g(r)$ is computed in a simulation, it is done by creating a histogram of particle distances for a single simulation frame, resulting in a noisy function that is most often averaged over several frames.

Given $g(r)$ vs. r data for a single frame, you will train a decision tree regressor to represent the underlying function.

First, run the cell below to load the data, etc.:

```
In [1]: import numpy as np
import matplotlib.pyplot as plt
from sklearn.tree import DecisionTreeRegressor, plot_tree

r = np.array([0.008,0.024,0.04,0.056,0.072,0.088,0.104,0.12,0.136,0.152,0.168,0.184,0.2,0.216,0.232,0.248,0.264,0.28,0.296,0.312,0.328,0.344,0.36,0.376,0.392,0.408,0.424,0.44,0.456,0.472,0.488,0.504,0.52,0.536,0.552,0.568,0.584,0.6,0.616,0.632,0.648,0.664,0.68,0.696,0.712,0.728,0.744,0.76,0.776,0.792,0.808,0.824,0.84,0.856,0.872,0.888,0.904,0.92,0.936,0.952,0.968,0.984,1.0,1.016,1.032,1.048,1.064,1.08,1.096,1.112,1.128,1.144,1.16,1.176,1.192,1.208,1.224,1.24,1.256,1.272,1.288,1.304,1.32,1.336,1.352,1.368,1.384,1.4,1.416,1.432,1.448,1.464,1.48,1.496,1.512,1.528,1.544,1.56,1.576,1.592,1.608,1.624,1.64,1.656,1.672,1.688,1.704,1.72,1.736,1.752,1.768,1.784,1.8,1.816,1.832,1.848,1.864,1.88,1.896,1.912,1.928,1.944,1.96,1.976,1.992,2.008,2.024,2.04,2.056,2.072,2.088,2.104,2.12,2.136,2.152,2.168,2.184,2.2,2.216,2.232,2.248,2.264,2.28,2.296,2.312,2.328,2.344,2.36,2.376,2.392,2.408,2.424,2.44,2.456,2.472,2.488,2.504,2.52,2.536,2.552,2.568,2.584,2.6,2.616,2.632,2.648,2.664,2.68,2.696,2.712,2.728,2.744,2.76,2.776,2.792,2.808,2.824,2.84,2.856,2.872,2.888,2.904,2.92,2.936,2.952,2.968,2.984,3.0,3.016,3.032,3.048,3.064,3.08,3.096,3.112,3.128,3.144,3.16,3.176,3.192,3.208,3.224,3.24,3.256,3.272,3.288,3.304,3.32,3.336,3.352,3.368,3.384,3.4,3.416,3.432,3.448,3.464,3.48,3.496,3.512,3.528,3.544,3.56,3.576,3.592,3.608,3.624,3.64,3.656,3.672,3.688,3.704,3.72,3.736,3.752,3.768,3.784,3.8,3.816,3.832,3.848,3.864,3.88,3.896,3.912,3.928,3.944,3.96,3.976,3.992,4.008,4.024,4.04,4.056,4.072,4.088,4.104,4.12,4.136,4.152,4.168,4.184,4.2,4.216,4.232,4.248,4.264,4.28,4.296,4.312,4.328,4.344,4.36,4.376,4.392,4.408,4.424,4.44,4.456,4.472,4.488,4.504,4.52,4.536,4.552,4.568,4.584,4.6,4.616,4.632,4.648,4.664,4.68,4.696,4.712,4.728,4.744,4.76,4.776,4.792,4.808,4.824,4.84,4.856,4.872,4.888,4.904,4.92,4.936,4.952,4.968,4.984,5.0,5.016,5.032,5.048,5.064,5.08,5.096,5.112,5.128,5.144,5.16,5.176,5.192,5.208,5.224,5.24,5.256,5.272,5.288,5.304,5.32,5.336,5.352,5.368,5.384,5.4,5.416,5.432,5.448,5.464,5.48,5.496,5.512,5.528,5.544,5.56,5.576,5.592,5.608,5.624,5.64,5.656,5.672,5.688,5.704,5.72,5.736,5.752,5.768,5.784,5.8,5.816,5.832,5.848,5.864,5.88,5.896,5.912,5.928,5.944,5.96,5.976,5.992,6.008,6.024,6.04,6.056,6.072,6.088,6.104,6.12,6.136,6.152,6.168,6.184,6.2,6.216,6.232,6.248,6.264,6.28,6.296,6.312,6.328,6.344,6.36,6.376,6.392,6.408,6.424,6.44,6.456,6.472,6.488,6.504,6.52,6.536,6.552,6.568,6.584,6.6,6.616,6.632,6.648,6.664,6.68,6.696,6.712,6.728,6.744,6.76,6.776,6.792,6.808,6.824,6.84,6.856,6.872,6.888,6.904,6.92,6.936,6.952,6.968,6.984,7.0,7.016,7.032,7.048,7.064,7.08,7.096,7.112,7.128,7.144,7.16,7.176,7.192,7.208,7.224,7.24,7.256,7.272,7.288,7.304,7.32,7.336,7.352,7.368,7.384,7.4,7.416,7.432,7.448,7.464,7.48,7.496,7.512,7.528,7.544,7.56,7.576,7.592,7.608,7.624,7.64,7.656,7.672,7.688,7.704,7.72,7.736,7.752,7.768,7.784,7.8,7.816,7.832,7.848,7.864,7.88,7.896,7.912,7.928,7.944,7.96,7.976,7.992,8.008,8.024,8.04,8.056,8.072,8.088,8.104,8.12,8.136,8.152,8.168,8.184,8.2,8.216,8.232,8.248,8.264,8.28,8.296,8.312,8.328,8.344,8.36,8.376,8.392,8.408,8.424,8.44,8.456,8.472,8.488,8.504,8.52,8.536,8.552,8.568,8.584,8.6,8.616,8.632,8.648,8.664,8.68,8.696,8.712,8.728,8.744,8.76,8.776,8.792,8.808,8.824,8.84,8.856,8.872,8.888,8.904,8.92,8.936,8.952,8.968,8.984,9.0,9.016,9.032,9.048,9.064,9.08,9.096,9.112,9.128,9.144,9.16,9.176,9.192,9.208,9.224,9.24,9.256,9.272,9.288,9.304,9.32,9.336,9.352,9.368,9.384,9.4,9.416,9.432,9.448,9.464,9.48,9.496,9.512,9.528,9.544,9.56,9.576,9.592,9.608,9.624,9.64,9.656,9.672,9.688,9.704,9.72,9.736,9.752,9.768,9.784,9.8,9.816,9.832,9.848,9.864,9.88,9.896,9.912,9.928,9.944,9.96,9.976,9.992,10.008,10.024,10.04,10.056,10.072,10.088,10.104,10.12,10.136,10.152,10.168,10.184,10.2,10.216,10.232,10.248,10.264,10.28,10.296,10.312,10.328,10.344,10.36,10.376,10.392,10.408,10.424,10.44,10.456,10.472,10.488,10.504,10.52,10.536,10.552,10.568,10.584,10.6,10.616,10.632,10.648,10.664,10.68,10.696,10.712,10.728,10.744,10.76,10.776,10.792,10.808,10.824,10.84,10.856,10.872,10.888,10.904,10.92,10.936,10.952,10.968,10.984,11.0,11.016,11.032,11.048,11.064,11.08,11.096,11.112,11.128,11.144,11.16,11.176,11.192,11.208,11.224,11.24,11.256,11.272,11.288,11.304,11.32,11.336,11.352,11.368,11.384,11.4,11.416,11.432,11.448,11.464,11.48,11.496,11.512,11.528,11.544,11.56,11.576,11.592,11.608,11.624,11.64,11.656,11.672,11.688,11.704,11.72,11.736,11.752,11.768,11.784,11.8,11.816,11.832,11.848,11.864,11.88,11.896,11.912,11.928,11.944,11.96,11.976,11.992,12.008,12.024,12.04,12.056,12.072,12.088,12.104,12.12,12.136,12.152,12.168,12.184,12.2,12.216,12.232,12.248,12.264,12.28,12.296,12.312,12.328,12.344,12.36,12.376,12.392,12.408,12.424,12.44,12.456,12.472,12.488,12.504,12.52,12.536,12.552,12.568,12.584,12.6,12.616,12.632,12.648,12.664,12.68,12.696,12.712,12.728,12.744,12.76,12.776,12.792,12.808,12.824,12.84,12.856,12.872,12.888,12.904,12.92,12.936,12.952,12.968,12.984,13.0,13.016,13.032,13.048,13.064,13.08,13.096,13.112,13.128,13.144,13.16,13.176,13.192,13.208,13.224,13.24,13.256,13.272,13.2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.128,25.144,25.16,25.176,25.192,25.208,25.224,25.24,25.256,25.272,25.288,25.304,25.32,25.336,25.352,25.368,25.384,25.4,25.416,25.432,25.448,25.464,25.48,25.496,25.512,25.528,25.544,25.56,25.576,25.592,25.608,25.624,25.64,25.656,25.672,25.688,25.704,25.72,25.736,25.752,25.768,25.784,25.8,25.816,25.832,25.848,25.864,25.88,25.896,25.912,25.928,25.944,25.96,25.976,25.992,26.008,26.024,26.04,26.056,26.072,26.088,26.104,26.12,26.136,26.152,26.168,26.184,26.2,26.216,26.232,26.248,26.264,26.28,26.296,26.312,26.328,26.344,26.36,26.376,26.392,26.408,26.424,26.44,26.456,26.472,26.488,26.504,26.52,26.536,26.552,26.568,26.584,26.6,26.616,26.632,26.648,26.664,26.68,26.696,26.712,26.728,26.744,26.76,26.776,26.792,26.808,26.824,26.84,26.856,26.872,26.888,26.904,26.92,26.936,26.952,26.968,26.984,27.0,27.016,27.032,27.048,27.064,27.08,27.096,27.112,27.128,27.144,27.16,27.176,27.192,27.208,27.224,27.24,27.256,27.272,27.288,27.304,27.32,27.336,27.352,27.368,27.384,27.4,27.416,27.432,27.448,27.464,27.48,27.496,27.512,27.528,27.544,27.56,27.576,27.592,27.608,27.624,27.64,27.656,27.672,27.688,27.704,27.72,27.736,27.752,27.768,27.784,27.8,27.816,27.832,27.848,27.864,27.88,27.896,27.912,27.928,27.944,27.96,27.976,27.992,28.008,28.024,28.04,28.056,28.072,28.088,28.104,28.12,28.136,28.152,28.168,28.184,28.2,28.216,28.232,28.248,28.264,28.28,28.296,28.312,28.328,28.344,28.36,28.376,28.392,28.408,28.424,28.44,28.456,28.472,28.488,28.504,28.52,28.536,28.552,28.568,28.584,28.6,28.616,28.632,28.648,28.664,28.68,28.696,28.712,28.728,28.744,28.76,28.776,28.792,28.808,28.824,28.84,28.856,28.872,28.888,28.904,28.92,28.936,28.952,28.968,28.984,29.0,29.016,29.032,29.048,29.064,29.08,29.096,29.112,29.128,29.144,29.16,29.176,29.192,29.208,29.224,29.24,29.256,29.272,29.288,29.304,29.32,29.336,29.352,29.368,29.384,29.4,29.416,29.432,29.448,29.464,29.48,29.496,29.512,29.528,29.544,29.56,29.576,29.592,29.608,29.624,29.64,29.656,29.672,29.688,29.704,29.72,29.736,29.7
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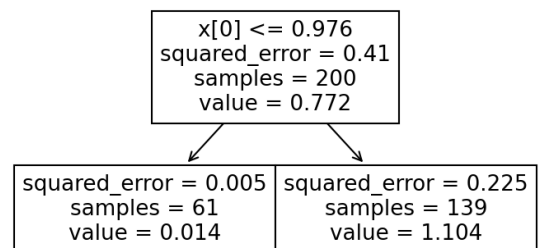
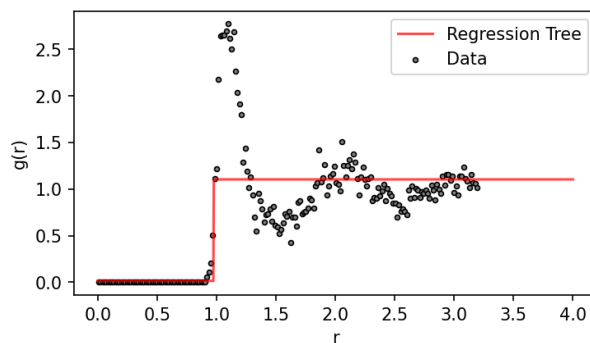
Training regression trees

For input `r` and output `g`, train a `DecisionTreeRegressor()` to perform the regression with `max_depth` values of 1, 2, 6, 10.

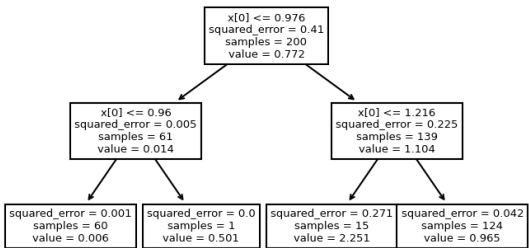
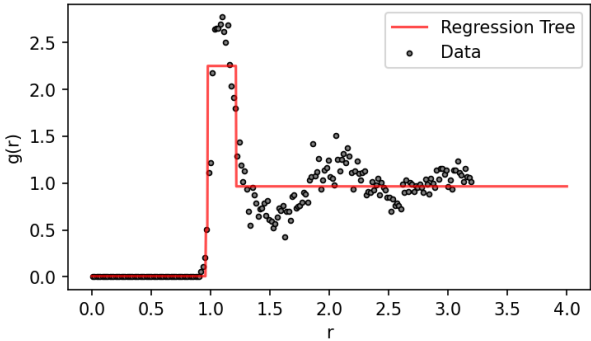
Complete the code below, which will plot your decision tree results and visualize the tree. Name each decision tree within the loop `dt`.

Note: you may need to resize the input `r` as `r.reshape(-1,1)` before passing it as input into the fitting function.

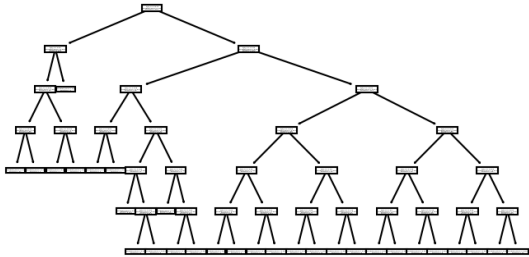
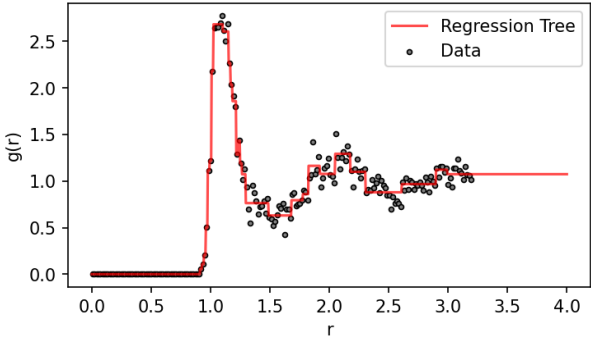
```
In [3]: for max_depth in [1, 2, 6, 10]:
# YOUR CODE GOES HERE
# Create and fit `dt`
dt = DecisionTreeRegressor(max_depth = max_depth)
dt.fit(r.reshape(-1,1),g)
plot(r,g,dt)
```



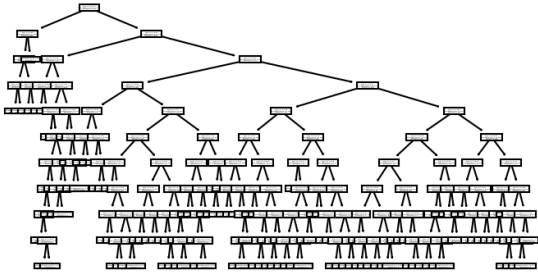
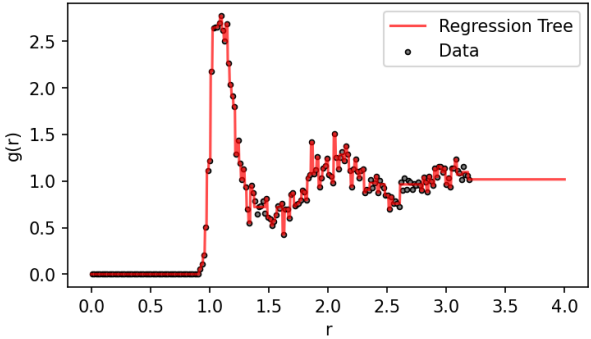
Tree max. depth: 1



Tree max. depth: 2



Tree max. depth: 6



Tree max. depth: 10

In []: